

On the sign structure of doped Mott insulators

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We demonstrate that the sign structure of the t-J model on a hypercubic lattice is entirely different from that of a Fermi gas, by inspecting the high temperature expansion of the partition function up to all orders, as well as the multi-hole propagator of the half-filled state and the perturbative expansion of the ground state energy. We show that while the fermion signs can be completely gauged away by a Marshall sign transformation at half-filling, the bulk of the signs can be also gauged away in a doped case, leaving behind a rarified “irreducible” sign structure that can be enumerated easily by counting exchanges of holes with themselves and spins on their real space paths. Such a sparse sign structure implies a mutual statistics for the quantum states of the doped Mott insulator.

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The progress in the understanding of the physics of strongly interacting electron systems has been strongly hindered by the infamous fermion minus sign problem rendering field theoretical and statistical physics methods to be ill behaved for fermions. The t-J model, catching the essence of the doped Mott insulators, is archetypical. Despite twenty years of concerted effort, inspired by its relevance towards the problem of high T_c superconductivity,[1] nothing is known rigorously about this model, except then for the one dimensional case. In fact, the other exception is the Mott-insulating state at half-filling, where the Hubbard projection turns the indistinguishable fermions into distinguishable spins, and the remnant signs of the unfrustrated spin problem can be gauged away by a Marshall sign transformation.[2] Upon doping, however, the fermion signs get active again but it is obvious that the sign structure has to be quite different from that of a Fermi gas, given that all signs disappear at half filling.

It is instructive to first specify the sign structure in a Fermi gas. In a path-integral formalism,[3] the partition function of a Fermi gas can be expressed as

$$Z_{\text{FG}} = \sum_c (-1)^{N_{\text{ex}}[c]} Z_0[c] \quad (1)$$

with each path c composed of a set of closed loops of the spatial trajectories of all fermions and $Z_0[c] > 0$. The sign structure is then governed by $(-1)^{N_{\text{ex}}[c]}$, with $N_{\text{ex}}[c] = N - N_{\text{loop}}[c]$ where $N = \sum_w w C_w(c)$ is the total number of fermions and $N_{\text{loop}}[c] = \sum_w C_w(c)$ the closed loop number, in which w denotes the number of fermions in a loop (also called the winding number[3] of the loop) and $C_w(c)$, the number of loops with a given w for a given path c .

Here we report our discovery of a remarkably sparse sign structure for the t-J model, which can be rigorously identified at arbitrary doping. Basically, we shall prove

that the partition function for the t-J model is given by

$$Z_{\text{t-J}} = \sum_c \tau_c \mathcal{Z}[c] \quad (2)$$

where $\mathcal{Z}[c] > 0$ [see (14)] and the sign structure

$$\tau_c \equiv (-1)^{N_h^\downarrow[c] + N_{\text{ex}}^h[c]} \quad (3)$$

for a given c composed of a set of closed loops for all holes and spins (an example is shown in Fig. 1), where $N_h^\downarrow[c]$ denotes the total number of exchanges between the holes and down spins and $N_{\text{ex}}^h[c]$ the total number of exchanges between holes. In addition to appearing in the above partition function, the sign structure τ_c will be also present in various physical quantities based on expansions in terms of quantum-paths in real space: the n -hole propagator of the Mott-insulating state as well as the zero temperature perturbation theory of the ground state energy (both up to all orders).

Compared to the full fermion signs in (1), which is an exactly solvable problem for a Fermi gas,[3] *the “sign problem” for the t-J model then becomes that τ_c in (3) is too sparse to be treated as a fermion perturbative problem.* It implies that in the mathematically equivalent slave-boson representation, the no double occupancy constraint must play a crucial role to “rarefy” the statistical signs of fermionic “spinons” in order to reproduce the correct sign structure τ_c , which disappears at half-filling. On the other hand, in the slave-fermion representation besides the statistical signs associated with the fermionic “holons” [related to N_{ex}^h in (3)], extra signs in τ_c will have to be generated *dynamically*, which are previously known as the phase strings identified in the one-hole case.[4]

In particular, we will show that in the two-dimensional (2D) case τ_c can be precisely captured by a pair of mutual Chern-Simons gauge fields: the electrical charges feel π flux-tubes attached to the spin “particles” and vice versa, in an all-boson formalism which is known as the phase string formulation derived before by a different

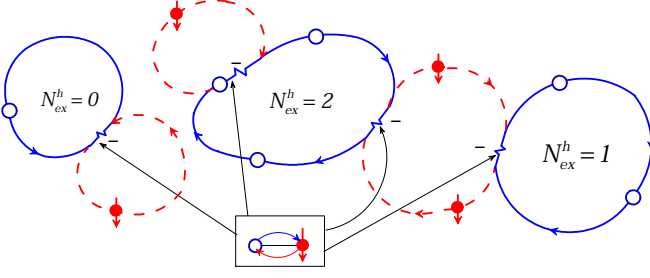


FIG. 1: A typical diagram for a set of closed paths, denoted by c in the expansion of the partition function given in (2). Only the hole and down spin loops are shown as the up spins are not independent due to the no double occupancy constraint. Pure spin loops without involving exchanges with the holes do not contribute to any signs and are not explicitly shown here. The total sign τ_c associated with the diagram, defined in (3), is determined by counting the hole-down-spin exchanges and the hole permutations. In this particular c , $N_h^{\downarrow} = 1 + 2 + 1 = 4$ and $N_{ex}^h = 0 + 2 + 1 = 3$ such that $\tau_c = -1$.

method.[5] So the unusual sign structure τ_c strongly hints a mutual statistics nature of this doped Mott insulator, and thus offers critical guidance in the construction of correct quantum states of it.

Let us begin with the t-J model on a bipartite lattice of any dimensions $H_{t-J} = H_t + H_J$. In the slave-fermion representation, the electron annihilation operator can be written as

$$c_{i\sigma} = (-\sigma)^i f_i^\dagger b_{i\sigma} \quad (4)$$

where f denotes the fermionic holon operator and b the bosonic spinon operator, which satisfy the no double occupancy constraint $f_i^\dagger f_i + \sum_\sigma b_{i\sigma}^\dagger b_{i\sigma} = 1$. Then the hopping and superexchange terms can be expressed, respectively, as follows

$$H_t = -t(P_{o\uparrow} - P_{o\downarrow}) \quad (5)$$

$$H_J = -\frac{J}{2}(P_{\uparrow\downarrow} + Q) \quad (6)$$

where

$$P_{o\uparrow} = \sum_{\langle ij \rangle} f_i^\dagger f_j b_{j\uparrow}^\dagger b_{i\uparrow} + H.c. \quad (7)$$

$$P_{o\downarrow} = \sum_{\langle ij \rangle} f_i^\dagger f_j b_{j\downarrow}^\dagger b_{i\downarrow} + H.c. \quad (8)$$

$$P_{\uparrow\downarrow} = \sum_{\langle ij \rangle} b_{i\uparrow}^\dagger b_{j\uparrow} b_{j\downarrow}^\dagger b_{i\downarrow} + H.c. \quad (9)$$

$$Q = \sum_{\langle ij \rangle} (n_{i\uparrow} n_{j\downarrow} + n_{i\downarrow} n_{j\uparrow}) \quad (10)$$

Here $P_{o\uparrow}$ and $P_{o\downarrow}$ denote the nearest neighbor hole-spin exchange operators, $P_{\uparrow\downarrow}$ the nearest neighbor spin-spin

exchange operator, while the Q term describes the potential energy between the nearest neighbor antiparallel spins.

Note that the Marshall sign[2] factor $(-\sigma)^i$ is explicitly introduced in (4) such that the superexchange term H_J acquires a total negative sign in front of the spin exchange and potential operators. Then one finds the matrix element $\langle \phi' | H_J | \phi \rangle \leq 0$ where $|\phi\rangle$ and $|\phi'\rangle$ denote the Ising spin basis $b_{i_1\sigma_1}^\dagger b_{i_2\sigma_2}^\dagger \dots |0\rangle$, which implies that the H_J term will not cause any sign problem. In particular, the ground state of H_J can be always written as

$$|\psi_0\rangle = \sum_\phi \chi_\phi |\phi\rangle \quad \text{with } \chi_\phi \geq 0 \quad (11)$$

which is true even at doped case so long as there is no hopping term.

Partition function. The nontrivial sign problem only arises when holes are doped into the system and allowed to hop. It can be traced to the sign difference between the hole-spin exchange operators, $P_{o\uparrow}$ and $P_{o\downarrow}$, in the hopping term (5) in addition to the sign problem associated with fermionic holons. By making the high-temperature series expansion of the partition function up to all orders

$$\begin{aligned} Z_{t-J} &= \text{Tr} \{ e^{-\beta H_{t-J}} \} = \sum_n \frac{(-\beta)^n}{n!} \text{Tr} \{ (H_{t-J})^n \} \\ &= \sum_n \frac{(\beta J/2)^n}{n!} \text{Tr} \left\{ \sum \dots \left(\frac{2t}{J} P_{o\uparrow} \right) \dots \right. \\ &\quad \left. \cdot P_{\uparrow\downarrow} \dots \left(-\frac{2t}{J} P_{o\downarrow} \right) \dots Q \dots \right\} \end{aligned} \quad (12)$$

and inserting the complete set

$$\sum_{\phi \{l_h\}} |\phi; \{l_h\}\rangle \langle \phi; \{l_h\}| = 1 \quad (13)$$

between the operators inside the trace (here $|\phi; \{l_h\}\rangle$ is an Ising basis with ϕ specifying the spin configuration and $\{l_h\}$ denoting the positions of holes), one can evaluate term by term of the expansion in (12). Because of the trace, the initial and final hole and spin configurations should be the same such that all contributions to Z_{t-J} can be characterized by closed loops of holes and spins although each of them can involve multi-holes or -spins as shown in Fig. 1.

Finally one arrives at the compact form given in (2) based on the above high-temperature expansion, with

$$\mathcal{Z}[c] = \left(\frac{2t}{J} \right)^{M_h[c]} \sum_n \frac{(\beta J/2)^n}{n!} \delta_{n, M_h + M_{\uparrow\downarrow} + M_Q} \quad (14)$$

in which $M_h[c]$ and $M_{\uparrow\downarrow}[c]$ represent the total steps of the hole and down spin ‘‘hoppings’’ along the closed loops for a given path c , and $M_Q[c]$ the total number of down

spins interacting with the nearest-neighbor up spins via the potential term Q in (6). Obviously $\mathcal{Z}[c] \geq 0$ in (14). Thus the nontrivial sign structure of the partition function Z_{t-J} in (2) is entirely captured by τ_c in (3) where $N_h^\downarrow[c]$ denotes the total number of exchanges between the holes and down spins [i.e., those actions taken via $P_{o\downarrow}$ in (5)] and $N_{\text{ex}}^h[c]$ the total number of exchanges between holes arising from the fermionic statistics of the holon operator f .

The expression (2) for the partition function clearly demonstrates that τ_c precisely depicts the irreducible sign structure *at arbitrary doping, temperature, and dimensions* for the t-J model on a bipartite lattice. In the following, we shall further illustrate how τ_c similarly appears in other physical quantities.

Multi-hole propagator. Define the multi-hole propagator

$$G(\{j_s\}, \{i_s\}; E) = \langle \psi_0 | c_{j_1\sigma_1}^\dagger c_{j_2\sigma_2}^\dagger \cdots G(E) \cdots c_{i_2\sigma_2} c_{i_1\sigma_1} | \psi_0 \rangle \quad (15)$$

where $|\psi_0\rangle$ is the *half-filling* ground state and

$$G(E) = \frac{1}{E - H_{t-J} + 0^+}. \quad (16)$$

One can make the following expansion which converges at $E < E_G$ (the multi-hole ground state energy):

$$G(E) = \frac{1}{E} \sum_n \left(\frac{H_{t-J}}{E} \right)^n = \frac{1}{E} \sum_n \sum \cdots \left(\frac{t}{-E} P_{o\uparrow} \right) \cdots \left(\frac{J}{-2E} P_{\downarrow\uparrow} \right) \cdots \quad (17)$$

and then insert the complete set (13) between the exchange operators. Similar to the evaluation of the partition function, denoting c as a given set of *open* paths connecting the hole configurations $\{i_s\}$ and $\{j_s\}$, with $|\psi_0\rangle$ expanded in terms of $|\phi\rangle$ [(11)], we find

$$G(\{j_s\}, \{i_s\}; E) = -\Lambda \sum_{\phi\phi'} \frac{\chi_\phi \chi_{\phi'}}{-E} \sum_c \tau_c W[c; E] \quad (18)$$

in which each set of paths c is weighed by the phase strings τ_c and an amplitude

$$W[c; E] = \left(\frac{t}{-E} \right)^{M_h} \left(\frac{J}{-2E} \right)^{M_{\uparrow\downarrow} + M_Q} \quad (19)$$

with $\Lambda = \prod_{s=1}^{N_h} (-\sigma_s)^{i_s - j_s}$. At $E < E_G < 0$, the expansion (18) is converged, and $W[c; E] \geq 0$ shows that τ_c is indeed an “irreparable” (irreducible) sign which is expected to play a critical role via constructive and destructive quantum phase interferences among different “path” c ’s. Note that the single-hole version of (15) has been previously discussed in Ref. [4, 5].

Ground state wave function. Define a wave function

$$\Psi_0[\mathcal{R}] \equiv \langle \psi_0 | c_{i_1\sigma_1}^\dagger c_{i_2\sigma_2}^\dagger \cdots | \Psi_0 \rangle \quad (20)$$

with $|\Psi_0\rangle$ as the true ground state and $\mathcal{R} \equiv \{i_h\}; \{\sigma_s\}$. Then, according to (15) and (16), $\Psi_0[\mathcal{R}]$ will be selected as $E \rightarrow E_G$ from below, with (18) implying

$$\Psi_0(\mathcal{R}) \Psi_0^*(\mathcal{R}) \rightarrow \sum_{c_{\mathcal{R}}} \tau_{c_{\mathcal{R}}} \mathcal{W}[c_{\mathcal{R}}] \quad (21)$$

where on the right hand side the path $c_{\mathcal{R}}$ ’s are all the closed loops connected to \mathcal{R} , each weighed by a positive amplitude $\mathcal{W}[c_{\mathcal{R}}] = \sum_{\phi\phi'} \chi_\phi \chi_{\phi'} W[c_{\mathcal{R}}; E] \frac{E - E_0}{E_0} \Big|_{E \rightarrow E_0}$. Therefore the sign structure $\tau_{c_{\mathcal{R}}}$ must be naturally built into the ground state wave function. In the following we first examine the ground state energy, and then the mutual statistics implied for the wave function.

Ground state energy. Based on the Goldstone’s theorem,[6] the energy shift of the ground state due to the hopping term H_t can be expressed by

$$E_G - \Omega_0 = \langle \Psi_0 | H_t \sum_{n=0}^{\infty} \left(\frac{1}{\Omega_0 - H_J} H_t \right)^n | \Psi_0 \rangle_{\text{connected}} \quad (22)$$

where $H_J |\Psi_0\rangle = \Omega_0 |\Psi_0\rangle$ and the subscript “connected” means that only matrix elements of the operator in (22) which start from the ground state $|\Psi_0\rangle$ and end with $|\Psi_0\rangle$ without disconnected parts should be included.

Here $|\Psi_0\rangle$ is generally written in a translational invariant form with a momentum \mathbf{K} :

$$|\Psi_0(\mathbf{K})\rangle = \sum_{\mathbf{R}} e^{i\mathbf{K} \cdot \mathbf{R}} |\Phi_0; \{\mathbf{r}_{l_h} - \mathbf{R}\}\rangle$$

where $|\Phi_0; \{\mathbf{r}_{l_h}\}\rangle$ is also the ground state of H_J for a set of hole distribution $\{\mathbf{r}_{l_h}\}$ which minimizes the superexchange energy Ω_0 . Like in the half-filling case, one can expand $|\Phi_0; \{\mathbf{r}_{l_h}\}\rangle$ in terms of the Ising basis: $|\Phi_0; \{\mathbf{r}_{l_h}\}\rangle = \sum_{\phi} \chi_{\phi}(\{\mathbf{r}_{l_h}\}) |\phi; \{\mathbf{r}_{l_h}\}\rangle$ with $\chi_{\phi} \geq 0$ as mentioned before.

By making the expansion in terms of H_J/Ω_0 and using a similar procedure in dealing with the expansion (17), one finally gets

$$E_G - \Omega_0 = \Omega_0 \sum_{\mathbf{R}\mathbf{R}'} e^{i\mathbf{K} \cdot (\mathbf{R} - \mathbf{R}')} \sum_{\phi\phi'} \chi_{\phi'} \chi_{\phi} \sum_{c(\text{connected})} \tau_c W[c; \Omega_0] \quad (23)$$

in which the path c starts from $|\Phi_0; \{\mathbf{r}_{l_h} - \mathbf{R}\}\rangle$ and ends with $|\Phi_0; \{\mathbf{r}_{l_h} - \mathbf{R}'\}\rangle$ without including the “disconnected” paths.[6] Indeed the sign factor τ_c , weighed by $W[c; \Omega_0] \geq 0$ defined in (19), determines the ground state energy shift upon doping.

Mutual statistics. τ_c in (3) suggests that statistics signs of the fermionic holes associated with the slave-fermion

representation are actually indistinguishable from the “phase strings” generated by the motion of holes. It will be thus instructive to treat the whole sign structure on an *equal footing*: take the holon and spinon mathematically as all *bosons* and redefine the hole-spin and spin-spin exchange operators (5) and (6) by

$$P_{o\uparrow} = \sum_{\langle ij \rangle} \left(e^{-iF_{ij}} h_i^\dagger h_j \right) \left(b_{j\uparrow}^\dagger b_{i\uparrow} \right) + H.c. \quad (24)$$

$$-P_{o\downarrow} = \sum_{\langle ij \rangle} \left(e^{-iF_{ij}} h_i^\dagger h_j \right) \left(e^{-iG_{ji}} b_{j\downarrow}^\dagger b_{i\downarrow} \right) + H.c. \quad (25)$$

$$P_{\uparrow\downarrow} = \sum_{\langle ij \rangle} \left(b_{i\uparrow}^\dagger b_{j\uparrow} \right) \left(e^{-iG_{ji}} b_{j\downarrow}^\dagger b_{i\downarrow} \right) + H.c. \quad (26)$$

where the fermionic holon f_i is replaced by a *bosonic* h_i and the minus sign in front of $P_{o\downarrow}$ is absorbed. The Q term (10) remains unchanged. In 2D case, it is straightforward to verify that if F_{ij} and G_{ij} are chosen as

$$F_{ij} = \sum_{l \neq i,j} [\theta_i(l) - \theta_j(l)] (n_{l\downarrow}^b + n_l^h) \quad (27)$$

$$G_{ij} = \sum_{l \neq i,j} [\theta_i(l) - \theta_j(l)] n_l^h \quad (28)$$

where $n_{l\sigma}^b$ and n_l^h are the number operators of spinon (σ) and holon, respectively, and $\theta_i(l) = \Im \ln(z_i - z_l)$ with z_i denoting the complex coordinate of site i , then the partition function (2) can be correctly reproduced. Without F_{ij} and G_{ij} , by contrast, one finds $\tau_c \equiv 1$ in (2). Namely the sign structure is indeed entirely captured by the phase factors, $e^{-iF_{ij}}$ and $e^{-iG_{ji}}$, in this bosonic formalism.

Rewriting $F_{ij} \equiv -A_{ij}^s + \phi_{ij}^0 + A_{ij}^h$, and $G_{ij} \equiv 2A_{ij}^h$, and using the constraint $\sum_{\sigma} n_{l\sigma}^b + n_l^h = 1$, one can show that the three link variables, A_{ij}^s , A_{ij}^h , and ϕ_{ij}^0 , satisfy $\sum_{\Gamma} A_{ij}^s = \pm\pi \sum_{l \in \Sigma_{\Gamma}} (n_{l\uparrow}^b - n_{l\downarrow}^b)$, and $\sum_{\Gamma} A_{ij}^h = \pm\pi \sum_{l \in \Sigma_{\Gamma}} n_l^h$, for a loop Γ enclosing an area Σ_{Γ} , and $\sum_{\square} \phi_{ij}^0 = \pm\pi$ for each plaquette. So they describe π flux tubes bound to spinons, holons, and each plaquette, respectively. Since the Hamiltonian is invariant under gauge transformations $h_i \rightarrow h_i e^{i\varphi_i}$, $A_{ij}^s \rightarrow A_{ij}^s + (\varphi_i - \varphi_j)$ and $b_{i\sigma} \rightarrow b_{i\sigma} e^{i\sigma\theta_i}$, $A_{ij}^h \rightarrow A_{ij}^h + (\theta_i - \theta_j)$, the bosonic holons and spinons carry the gauge charges of A_{ij}^s and A_{ij}^h , respectively. With the effect of τ_c described by the mutual Chern-Simons gauge fields, A_{ij}^s and A_{ij}^h , the t-J model in the bosonic formalism explicitly becomes a mutual fractional statistics (mutual semions) problem.[5] Correspondingly, the electron wave function ψ_e of the t-J model can be also expressed in terms of ψ_b in this bosonic formalism via $\psi_e = \mathcal{K}\psi_b$, [7] in which the large gauge transformation \mathcal{K} will transform by

$$\mathcal{K} \longrightarrow \tau_c \mathcal{K} \quad (29)$$

under an operation that the hole and spin coordinates are continuously permuted via a series of nearest neigh-

bor exchanges (with the no double occupancy obeyed at each step), with the coordinates forming closed loops, denoted by c , after the system back to the original configuration at the end of the operation. By comparison, the sign structure in (1) is related to the usual antisymmetric fermionic wave functions for a Fermi gas.

In summary, we have demonstrated rigorously that the Hubbard projections inherent to the physics of doped Mott insulators change the rules of fermion statistics fundamentally as compared to the Fermi gas. Pending the doping level, the irreducible sign structure that is of relevance to the physics is much more sparse in the former and we have shown that at least in real space expansions these irreducible signs are easy to count. In particular, in the 2D case, we have established a precise relation in which the physical sign structure of the t-J model is explicitly determined by the mutual Chern-Simons fields, with the wave function satisfying the mutual statistics.

This does not mean that we have solved the problem – the “mutual Chern-Simons” theory[8] of the phase string formulation is still far from being completely understood. However, our results open up new alleys for investigation. High temperature expansions should be revisited to study in detail in what regard the t-J signs differ from those of a Fermi gas. It would be quite interesting to find out how the “irreducible” hyper nodal surfaces of numerically determined $t-J$ model ground states look like. At the least, it seems possible to critically test Anderson’s conjecture[9] that the ground state of the doped Mott-insulator has to be orthogonal to that of the Fermi liquid, using the elementary fact that wave functions having a qualitatively different nodal surface cannot overlap.

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